

CURRICULUM VITAE

Wenqing Zhang (张文清)

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Title

Professor of Materials Physics

Research Interests

- Energy conversion materials: thermoelectrics and photovoltaics;
- Interfaces in ceramics, interface-related phenomena and microstructure evolution of materials;
- Materials Physics; optical, electrical and thermal properties; materials at reduced dimensions;
- Computational materials science; materials design from *ab initio*, multiscale materials simulations;
- Close cooperation with experimentalists on thermoelectric and photovoltaic research.

Education

Ph.D. in Physics (1992), Shanghai Institute of Optics and Fine Mechanics,
Chinese Academy of Sciences, China

M.Sc.(1986) and B.Sc. (1989) in Physics, Department of Physics, Xiamen University, China

Professional Experience

Professor (2003.12 -- present)

Shanghai Institute of Ceramics, Chinese Academy of Sciences,
1295 Dingxi Road, Shanghai, 200050, China

Visiting Professor (2004.7-8; 2005.2-3)

Institute for Metal Research, Max-Planck-Gesellschaft, Stuttgart, Germany

Research Faculty (2002.6 – 2003.12)

Materials Department, University of California, Santa Barbara, Santa Barbara, CA 93106

Research Staff (1999.12 –2002.5)

Princeton Materials Institute, Princeton University, Princeton, NJ 08540

Research Associate Fellowship (1997.12 – 1999.11)

Division of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138

Visiting Scientist (1997.7 – 1997.12)

Theory Department, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin-Dahlem, Germany

Associate Professor (1995.5 – 1997.6)

Institute of Applied Physics, Beijing University of Science & Technology, China

Postdoctoral Researcher (1993.1 -- 1995.3)

Institute of Physics, Chinese Academy of Science, China (王鼎盛 研究员)

Methods Used for Research

- *Ab initio* methods based on density-functional theory, pseudopotential plane wave and full-potential linearized augmented plane-wave methods;
- LDA+U and GW methods for excited states of solids;
- Molecular dynamics and multiscale materials simulations for complex materials phenomena.

Selected Professional Activities

- **Symposium Co-Organizer** for:
 - ✧ Co-Chair: Symposium on “*Engineering Interfaces for New Materials: Modeling and Experiments*”, Annual Meeting of the Physical Society of America (APS’2008), New Orleans, March 2008
 - ✧ Chair: Symposium on “*Thermoelectric Materials and Devices*”, the 7th Pacific-rim Conference on Advanced Ceramics, Shanghai, China, Nov., 2007.
 - ✧ Co-chair: Symposium on “*Fundamental Research on Energy-conversion Materials*”, the 5th annual meeting of the Overseas Chinese Physics Association (OCPA5), Taipei, China, June., 2006.
 - ✧ Co-chair, Forum on “*Advanced Thermoelectric Materials and Devices*”, the 1st Shanghai International Forum on Advanced Materials, Shanghai, Nov. 2007.
 - ✧ Chair, Workshop on “*Thermoelectric Transport Fundamentals*”, the 2nd Shanghai International Workshop on High-performance Ceramics, Hangzhou, May. 2010.
- **Reviewer of Peer-reviewed Journals:** Phys. Rev. Lett., J. Am. Chem. Soc., Adv. Mater., Phys. Rev. B, Acta Mater., Appl. Phys. Lett., J. Appl. Phys., J. Elec. Mater. etc.

Current Research Grants

- 2008-2012, NSFC project under A3 foresight program (China-Japan-Korea A3 international cooperation project), *High-efficiency Nanostructured Thermoelectric Materials*.
- 2008-2012, NSFC special grant for exceptional young scientist (国家杰出青年基金), *Computational Materials Science and multiscale design for energy conversion materials*;
- 2007-2011, National Basic Research Program of China (973), *Electrical/Thermal Transport Fundamentals and Design Principles for Novel Thermoelectric Materials* ;
- 2007-2009, NSFC grant, *Ab initio Study on the Thermoelectric Properties of Multi-filled CoSb₃*;
- 2007-2010, NSFC key project, *Methodology Development of Electronic Structure and Transport Property Calculations for Correlated Systems – Electrical Transport Property of Thermoelectric Compounds* ;
- 2007-2009, CAS knowledge-innovation exploratory project, *Computational Materials Science* ;
- 2004-2008, CAS ‘One-hundred-talent plan (百人计划)’, *Computational Materials Physics* ;
- 2005-2007, NSFC grant, *Ab initio Study on the Adhesion Property of Metal-ceramic Interfaces* ;
- 2007-2010, International Cooperation Projects, General Motors R&D, Corning R&D, etc.;

Citation Statistics of Recent Publications (as of 2008):

SCI citations of work: > 800

Selected Publications (partial list)

--- More than 80 SCI papers published in Phys. Rev. Lett., Phys. Rev. B, J. Am. Chem. Soc., Adv. Funct. Mater., Appl. Phys. Lett., Acta Mater. etc.

1. Lili Xi, Jiong Yang, Caifei Lu, Zhigang Mei, Wenqing Zhang*, and Lidong Chen, “Systematic Study of the Multiple-Element Filling in Caged Skutterudite CoSb_3 ”, **Chem. Mater.**, DOI: 10.1021/cm903717w (2010).
2. X. Shi, J. Yang, S. Bai, Jihui Yang, H. Wang, M. Chi, J. R. Salvador, W. Zhang*, L. Chen, W. Wong-Ng, “On the Design of High-Efficiency Thermoelectric Clathrates through a Systematic Cross-Substitution Framework Elements”, **Adv. Funct. Mater.**, 20, 755,(2010).
3. Yongcheng Liang, Wenqing Zhang, Jianzhi Zhao et al, *Superhardness, stability, and metallicity of diamondlike BC5: Density functional calculations*. **Phys. Rev. B** 80, 113401 (2009).
4. Yongcheng Liang, Chun Li, Wanlin Guo, Wenqing Zhang, *First-principles investigation of technetium carbides and nitrides*, **Phys. Rev. B** 79, 024111 (2009).
5. SQ Bai, YZ Pei, LD Chen, W Zhang et al., *Enhanced thermoelectric performance of dual-element-filled skutterudites $\text{BaxCeyCo}_4\text{Sb}_{12}$* , **Acta. Mater.** 57, 3135-3139 (2009).
6. HT Li, W Zhang et al., *Ab Initio Thermodynamic Study of the Structure and Chemical Bonding of $\beta\text{-Ni}_{1-x}\text{Al}_x/\alpha\text{-Al}_2\text{O}_3$ Interface*, **Phys. Rev. B**, 80, 205422 (2009).
7. YZ Pei, LD Chen, W Zhang et al., *Improving Thermoelectric Performance of Caged Compounds through Light-element Filling*, **Appl. Phys. Lett.** (2009).
8. L Xi, J Yang, W Zhang, LD Chen et al., *Anomalous Dual-Element Filling in Partially Filled Skutterudites*, **J. Am. Chem. Soc.**, 131, 5560(2009).
9. J. Yang, L Xi, W Zhang, LD Chen, and Jihui Yang, *Electrical transport properties of filled CoSb_3 skutterudites: a theoretical study*, **J. Electron Mater.**, (2009).
10. J. Yang, HM. Li, T. Wu, W. Zhang et al., *Evaluation of Half-Heusler Compounds as Thermoelectric Materials: A theoretical Approach*, **Adv. Funct. Mater.**, 18, 2880(2008).
11. Shi X, Zhang W, Chen LD, and Yang J, *Thermodynamic Analysis of the Filling Fraction Limits for Impurities in CoSb_3 based on Ab initio calculations*, **Acta Mater.** 56, 1733(2008).
12. Shi X, Zhang W, Chen, LD and Uher C, *Phase-diagram-related Problems in Thermoelectric Materials: Skutterudites as an Example*, **Int. J. Mater. Res.** (formerly: Zeitschrift fuer Metallkunde), (2008).
13. Mei ZG, Jiong Yang, Zhang W, Chen LD et al., *Alkali-metal-filled CoSb_3 skutterudites as thermoelectric materials: Theoretical study*, **Phys. Rev. B** 77, 045202 (2008).
14. PEA Turchia, IA. Abrikosov, B Burton, SG. Friesd, G Grimvalle, L Kaufman, P Korzhavyie, V. RaoMangag, M Ohnoh, A Pisch, A Scottj, W Zhang, *Interface between quantum -mechanical -based approaches, experiments, and CALPHAD methodology*, **Calphad**, 31, 4-27(2007). This is a group review paper and I sponsored the writing of the *ab initio* part.
15. X. Shi, Z. Zhou, W. Zhang, L. D. Chen et al., *Solid solubility of Ir and Rh at the Co sites of skutterudites*, **J. Appl. Phys.** 101, 123525 (2007)
16. Y Du, J Wang, W Zhang et al., *Reassessment of the Al-Mn system and a thermodynamic description of the Al-Mg-Mn system*, **Int. J. Mat. Res.** 98, 855 (2007)
17. J. Yang, W. Zhang, S. Q. Bai, Z. Mei, and L. D. Chen, *Dual-frequency resonant phonon scattering in $\text{Ba}_x\text{R}_y\text{Co}_4\text{Sb}_{12}$ ($R=\text{La, Ce, and Sr}$)*, **Appl. Phys. Lett.** 90, 192111 (2007)

18. X. Shi, W. Zhang, L. D. Chen et al., *Theoretical study of the filling fraction limits for impurities in CoSb₃*, **Phys. Rev. B**, **75**, 235208 (2007).
19. Bo Wu, M Zinkevich, F. Aldinger and W. Zhang, *Ab initio structural and energetic study of LaMO₃ (M = Al, Ga) perovskites*, **J. Phys. Chem. Solids**, 68,570 (2007)
20. J Yang, W Zhang, *Structural stability of Se and Te nanowires*, **Acta Phys. Sin.** 56, 4107 (2007)
21. W. Zhang, *Reconstruction and structural transition at metal/diamond interfaces*, **Int. J. Mat. Res.** (formerly: Zeitschrift fuer Metallkunde) 97, 768 (2006).
22. JW Feng, W Zhang, et al., *Interfaces between Al₂O₃ and β -Ni_{1-x}Al_x alloy: Complex structures and ab initio thermodynamics*, **Phys. Rev. Lett.** **97**, 246102 (2006).
23. ZG Mei, W Zhang, LD Chen et al., *Filling Fraction Limits for Rear-earth metals in CoSb₃: An ab initio approach*, **Phys. Rev. B**74, 153202 (2006).
24. X. Y. Zhao, X. Shi, L. D. Chen, W. Zhang, S. Q. Bai, Y. Z. Pei, X. Y. Li, T. Goto, *Synthesis of Yb₃Co₄Sb₁₂/Y₂O₃ composites and their thermoelectric properties*, **Appl. Phys. Lett.** 89, 092121 (2006).
25. J. L. Zhao, W. Zhang et al., *Convergence of the formation energies of intrinsic point defects in wurtzite ZnO: first-principles study by projector augmented wave method*, **J. Phys.: Condens. Matter** 18, 1495 (2006).
26. Y. Z. Pei, L. D. Chen, W. Zhang, X. Shi, S. Q. Bai, X. Y. Zhao, Z. G. Mei, X. Y. Li, *Synthesis and thermoelectric properties of K_yCo₄Sb₁₂*, **Appl. Phys. Lett.** 89, 221107 (2006).
27. W Zhang, X. Shi, ZG Mei, LD Chen et al., *Prediction of ultrahigh filling fraction limit for K in CoSb₃*, **Appl. Phys. Lett.** (2006).
28. X. Shi, W. Zhang, LD Chen, J. Yang, *Filling Fraction Limit for Intrinsic Voids in Crystals: Doping in Skutterudites*, **Phys. Rev. Lett.** (2005).
29. J. Feng, W. Zhang, W. Jiang, *Study on the Ag/Al₂O₃ and Au/Al₂O₃ interfaces*, **Phys. Rev. B** (2005).
30. Y. Long Y, NX Chen NX, W Zhang, *Pair potentials for a metal-ceramic interface by inversion of adhesive energy*, **J. Phys.: Condens. Matter** 17, 2045 (2005).
31. M Zhou, LD Chen, W Zhang et al., *Disorder scattering effect on the high-temperature lattice thermal conductivity of TiCoSb-based half-Heusler compounds*, **J. Appl. Phys.**, 98, 013708 (2005).
32. W. Zhang, J. R. Smith, X.-G. Wang, *Thermodynamics from ab initio computations*, **Phys. Rev. B** **70**, 024103 (2004).
33. W. Zhang, J. R. Smith, and A. G. Evans, *Influence of Sulfur on the Adhesion of the Nickel/Alumina Interface*, **Phys. Rev. B**67, 245414(2003).
34. W. Zhang, J. R. Smith, and A. G. Evans, *The Connection Between Ab-initio Calculations and Interface Adhesion Measurements on Metal/oxide Systems: Ni/Al₂O₃ AND Cu/Al₂O₃*, **Acta Mater.**, 50, 3803 (2002).
35. W. Zhang, and J. R. Smith, *Nonstoichiometric interfaces and Al₂O₃ adhesion with Al and Ag*, **Phys. Rev. Lett.** 85,3225 (2000).
36. J. R. Smith, W. Zhang, *Stoichiometric interfaces of Al and Ag with Al₂O₃*, **Acta Mater**, 48, 4395(2000)..
37. W. Zhang, J.R. Smith, *Structure and adhesion of Nb/alpha-Al₂O₃ interface*, **Phys. Rev. B** 61, 16883(2000).

38. W. Zhang, and J. R. Smith, *Adhesion with Impurities: A Large Asymmetry*, **Phys. Rev. Lett.** 82, 3105(1999).
39. W. Zhang, E. Ma, *Magnetism and volume expansion of supersaturated Fe-Cu solid solutions: Ab-initio calculations compared with experiments*, **J. Mater. Res.**, 15, 653(2000).

Patents

1. J Yang, W Zhang, LD Chen , *Potassium and Sodium Filled Skutterudites*, **US Patent** , WO08008638 A2 (2008).
2. J Yang, LD Chen, W Zhang, and SQ Bai, X Shi and C Uher, *High Efficiency Skutterudite Type Thermoelectric Materials and Devices*, **US Patent**, Application # 61036715 (2008).
3. X Shi, J Yang, W Zhang et al., *Thermoelectric material including a multiple transition metal-doped type-I clathrate crystal structure*, **US Patent**, submitted (2009).
4. X Shi, J Yang, L Chen, W Zhang et al., *Thermoelectric material including a multiple-filled skutterudite crystal structure*, **US Patent**, submitted (2009).

Invited talks (partial list)

1. Invited talk on International Conference on Thermoelectrics, May 30-June 3, 2010, Shanghai, China.
2. Plenary talk on USA DOE workshop on thermoelectric materials, *Research on Thermoelectric Materials and Devices in China* , 2009.09.29-10.02, San Diego, CA, USA;
3. Invited talk on MS&T'07, *Filled CoSb₃ Thermoelectric Materials: from single to multiple filling* Pittsburgh. USA, Oct., (2008)
4. Keynote lecture on the 16th International conference on composite materials, *Modeling ceramic-metal interface from theory* , Kunming, China, July(2008).
5. Invited talk for Shanghai International Forum on Advanced Materials (SIFAM'2008) *Functionality of Interfaces*, Shanghai, Apr. (2009).
6. Keynote lecture on ISETS07, symposium on energy-conversion materials, *Thermoelectric material research in China*, Nagoya, Japan, Nov. (2007).
7. Invited talk on Asian10 conference on electronic structure calculations, *Rational Search for new thermoelectric Materials*, Hiroshima, Japan, Oct.(2007).
8. Invited talk on China-Sweden workshop on quantum simulations, *Thermoelectric Materials*, Gotheberg, Sweden, Aug.(2007).
9. Invited talk on China-Germany workshop on phase-diagram modeling, *Phase-diagram related problems in thermoelectric materials research*, Changsha, China, June(2007).
10. Invited talk on APS'07 March meeting, *Searching for new Thermoelectric Materials from Theory*. Denver. CO, March (2007).
11. Invited talk on the annual meeting of the America Ceramic Society (Daytona Beach), symposium on thermoelectric materials, *Thermoelectric material research in China*, Daytona Beach, USA. Jan. (2007).
12. Invited talk on China-Japan CAS-NEDO-AIST workshop on energy-conversion materials, *thermoelectric materials research*, Beijing, China, Dec.(2007).
13. Plenary talk on China-Japan meeting on phase-diagram calculations and materials design, *Modeling complex interfaces from theory*, Xiamen, China, Dec. (2006).

14. Invited talk for MRS'05 fall meeting, *Filling Fraction Limit for Impurities in CoSb₃: Physical Understanding and Insight for New Thermoelectric Materials*, Boston, USA, Dec. (2005).
15. Plenary lecture for the International Workshop on Thermodynamic Modeling and First-Principles Calculations, *Ab Initio Thermodynamics and Theoretical Study on Metal/Ceramic Interfaces*, Ringberg Castle Tegernsee, Germany, March (2005).
16. Invited talk for international workshop on Nano-interface Mechanics, *Interfaces with Ceramics: From ab-initio Calculations to Thermodynamics*, Tokyo, Japan, Sep. (2004).
17. Invited talk for American Physics Society (APS) meeting. See also Bulletin of the APS, 48, Part I, 301, *Pseudopotential Computations for Metal/Alumina Interfaces*, Austin, TX, March (2003).